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(FILE 'HOME' ENTERED AT 21:48:59 ON 24 SEP 2008)

FILE 'CA' ENTERED AT 21:49:07 ON 24 SEP 2008

L1 799 S CALIBRAT?(5A)TRANSFER?
L2 172 S L1 AND(VALIDAT? OR TRANSFER?)(3A)(SAMPLE OR SET OR STANDARD)
L3 29 S L1 AND(PRIMARY OR BASE OR FIRST)(4A)CALIBRAT?
L4 26 S L1 AND(SECOND? OR MODIF? OR UPGRAD?)(4A)CALIBRAT?
L5 289 S L1 AND (SPECTROMET? OR SPECTROSCOP? OR SPECTROPHOTOMETER OR
PHOTOMETER OR COLORIMETER OR ANALY!ER)
L6 92 S L2-4 AND L5
L7 13 S L1 AND STANDARDI?(3A)(SAMPLE OR SET)
L8 3 S L1 AND INDEPENDENT/TI
L9 102 S L6-8
L10 76 S L9 AND PY<2004
L11 1 S L9 NOT L10 AND PATENT/DT
L12 77 S L10-11
L13 25 S L9 NOT L12

=> d bib,ab 112 1-77

L12 ANSWER 5 OF 77 CA COPYRIGHT 2008 ACS on STN

AN 139:304090 CA

TI Multivariate calibration standardization across instruments for the
determination of glucose by Fourier transform near-infrared spectrometry

AU Zhang, Lin; Small, Gary W.; Arnold, Mark A.

CS Center for Intelligent Chemical Instrumentation, Department of Chemistry
and Biochemistry, Clippinger Laboratories, Ohio University, Athens, OH,
45701, USA

SO Analytical Chemistry (2003), 75(21), 5905-5915

AB The transfer of multivariate calibration models is investigated between
a primary (A) and two secondary Fourier transform near-IR (near-IR)
spectrometers (B, C). The application studied in this work is the use
of bands in the near-IR combination region of 5000-4000 cm⁻¹ to det.
physiol. levels of glucose in a buffered aq. matrix contg. varying
levels of alanine, ascorbate, lactate, triacetin, and urea. The three
spectrometers are used to measure 80 samples produced through a
randomized exptl. design that minimizes correlations between the
component concns. and between the concns. of glucose and water. Direct
standardization (DS), piecewise direct standardization (PDS), and guided
model reoptimization (GMR) are evaluated for use in transferring partial
least-squares calibration models developed with the spectra of 64
samples from the primary instrument to the prediction of glucose concns.
in 16 prediction samples measured with each secondary spectrometer. The
three algorithms are evaluated as a function of the no. of
standardization samples used in transferring the calibration models.
Performance criteria for judging the success of the calibration transfer
are established as the std. error of prediction (SEP) for internal
calibration models built with the spectra of the 64 calibration samples
collected with each secondary spectrometer. These SEP values are 1.51
and 1.14 mM for spectrometers B and C, resp. When calibration
standardization is applied, the GMR algorithm is obsd. to outperform DS
and PDS. With spectrometer C, the calibration transfer is highly

successful, producing an SEP value of 1.07 mM. However, an SEP of 2.96 mM indicates unsuccessful calibration standardization with spectrometer B. This failure is attributed to differences in the variance structure of the spectra collected with spectrometers A and B. Diagnostic procedures are presented for use with the GMR algorithm that forecasts the successful calibration transfer with spectrometer C and the unsatisfactory results with spectrometer B.

L12 ANSWER 12 OF 77 CA COPYRIGHT 2008 ACS on STN

AN 137:152006 CA

TI Methods and apparatus for spectroscopic calibration model transfer

IN Thomas, Edward V.; Rowe, Robert K.; Haass, Michael J.

PA Rio Grande Medical Technologies, Inc., USA; Sandia Corporation

SO U.S., 34 pp., Cont.-in-part of U.S. Ser. No. 415,432.

PI US 6441388 B1 20020827 US 2000-563865 20000503

US 6157041 A 20001205 US 1999-415432 19991008

PRAI US 1998-170022 B2 19981013

US 1999-415432 A2 19991008

US 2000-563865 A 20000503

US 2000-672326 A2 20000928

AB The invention concerns a method and app. for measuring a biol. attribute, such as the concn. of an analyte, particularly a blood analyte in tissue such as glucose. The method utilizes spectrog. techniques in conjunction with an improved instrument-tailored calibration model. In a calibration phase, calibration model data is modified to reduce or eliminate instrument-specific attributes, resulting in a calibration data set modeling intra-instrument variation. In a prediction phase, the prediction process is tailored for each target instrument sep. using a minimal no. of spectral measurements from each instrument. Diagrams describing the app. assembly and operation are given.

L12 ANSWER 14 OF 77 CA COPYRIGHT 2008 ACS on STN

AN 135:121425 CA

TI The transfer of fatty acid calibration equations using four sets of unsealed liquid standardisation samples

AU Garcia-Olmo, Juan; Garrido-Varo, Ana; De Pedro, Emiliano

CS Department of Animal Production, Faculty of Agriculture and Forestry Engineering, University of Cordoba, Cordoba, E-14080, Spain

SO Journal of Near Infrared Spectroscopy (2001), 9(1), 49-62

AB A database of 352 near IR (NIR) spectral data from Iberian pig liq. fat was used for the prediction of palmitic, stearic, oleic and linoleic fatty acids content. The results showed the excellent accuracy of NIR equations with coeffs. of detn. (r^2) reaching values close to 1 and std. error of cross-validation (SECV) values similar to the std. error in the ref. method (SEL). The possibility of transferring the calibrations developed in one instrument to another NIR instrument, following the Shenk and Westerhaus standardization algorithm, was examd. Two monochromator instruments were optically matched using four different standardization sets of unsealed samples (Set A: one sample of Iberian pig liq. fat with a similar fatty acids compn. to the av. of the calibration set; Set B: 20 samples of Iberian pig liq. fat covering the range in optical d. and fatty acid compn. of the calibration set; Set C:

oleic acid; Set D: linoleic acid). The standardization completed with Set A and Set B produced spectra on the satellite instrument which resembled spectra scanned on the master instrument. The std. error of the differences (SED) between the values predicted by the master and the satellite after standardization were similar to, or even lower than, the std. error of prediction (SEP) values for the same samples scanned on the master instrument.

L12 ANSWER 21 OF 77 CA COPYRIGHT 2008 ACS on STN

AN 132:168069 CA

TI Intersite transfer of industrial calibration models

AU Despagne, Frederic; Massart, D. Luc; Jansen, Martin; Van Daalen, Hans
CS ChemoAC, Pharmaceutical Institute, Vrije Universiteit Brussel, Brussels, B-1090, Belg.

SO Analytica Chimica Acta (2000), 406(2), 233-245

AB Two instrument standardization methods, the piecewise direct standardization and a method based on neural networks, are compared for the transfer of industrial near-IR powder spectra between two sites. Some important issues that can affect transfer, such as influence of signal preprocessing or representativity of standardization samples are discussed in detail. Particularities and limitations specific to each transfer method are outlined. In particular, it is shown that both methods lead to different reconstruction results in the presence of structured background noise.

L12 ANSWER 42 OF 77 CA COPYRIGHT 2008 ACS on STN

AN 125:237086 CA

OREF 125:44003a,44006a

TI A method for standardizing a spectrometer

IN Villemoes, Andersen Hans; Kjaer, Lisa; Waaben, Hansen Per; Ridder, Carsten

PA Foss Electric A/s, Den.

SO PCT Int. Appl., 70 pp.

PI WO 9624832 A1 19960815 WO 1996-DK68 19960209

US 5933792 A 19990803 US 1996-624470 19960403

PRAI DK 1995-153 A 19950209

DK 1995-853 A 19950721

AB A method for standardizing a spectrometer generating an optical spectrum from a sample, comprising generating at least one optical spectrum from at least one standardization sample each having a chem. compn. resulting in the optical spectrum showing a characteristic pattern in a predetd. frequency range, comparing information relating to the pattern(s) to corresponding information relating to at least one ref. pattern previously defined as the desired std. response from the at least one standardization sample, detg., based on the comparison, standardizing parameters describing the transition of the pattern(s) of the generated spectrum or spectra to the ref. pattern(s) and storing said standardizing parameters in the spectrometer or a computer connected thereto, so that the spectrometer, when presented to an unknown sample, will, using the standardization parameters, generate an optical spectrum substantially identical to that which would be generated in a corresponding spectrometer standardized with a sample of the same chem. compn. using the same previously defined ref. pattern(s). The present

method relates to standardization of the instrument to a well-defined state into which any no. of instruments may be brought. In this state, calibrations may be transferred freely from instrument to instrument.

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